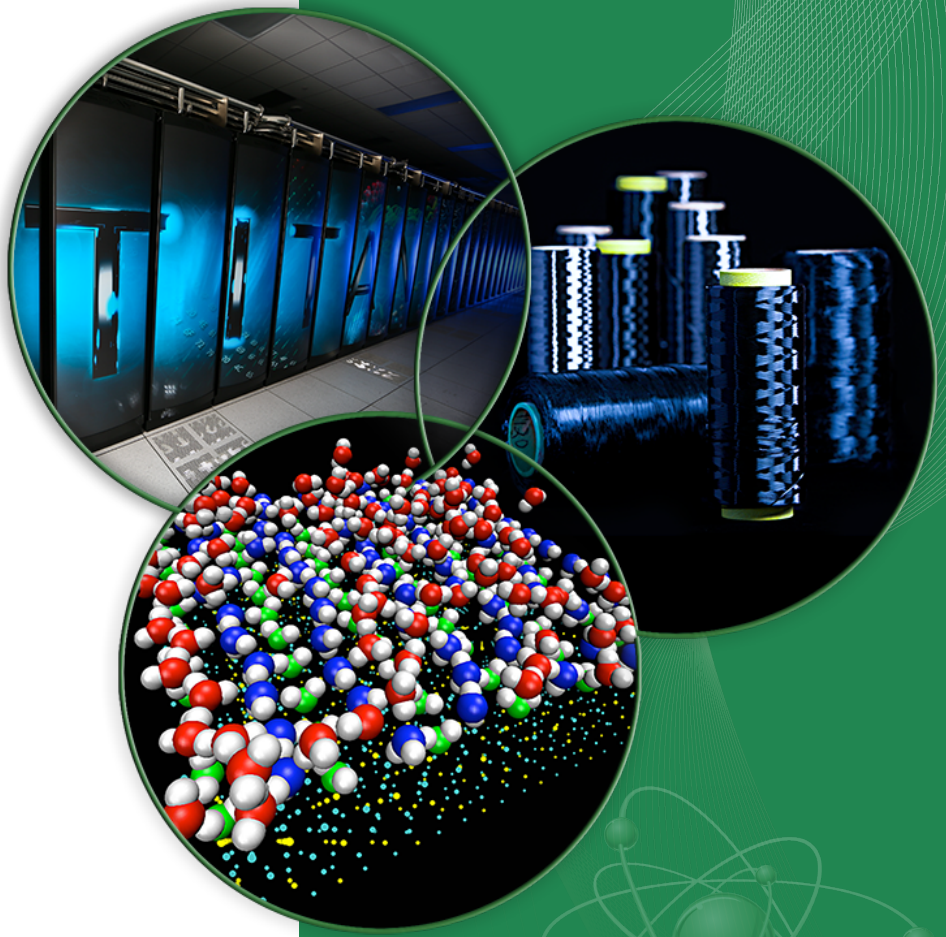
Cross Section Evaluation of ^{40}Ca for Neutron Energies up to 1.5 MeV and Validation of Tungsten Cross Sections up to 100 keV



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Sandia National Laboratories
Albuquerque, March 2016

Outline

- Motivation
- Nuclear data evaluation overview for ^{40}Ca
- Evaluation procedure with SAMMY
  - Channels definition
  - Experimental data overview
- Cross section evaluation work on ^{40}Ca (results)
- Validation work on $^{182\text{-}184,186}$W cross sections (results)
- Conclusions

Motivation

- **Calcium**
  - present in structural materials such as concrete and admixed material in waste streams
  - neutron-absorbing element that can influence the reactivity of systems with fissionable material
  - need for improved cross sections is identified specifically for *Hanford Plutonium Finishing plant* and *Hanford Tank Farms* in the DOE complex
  - Need for evaluated covariance data to support sensitivity/ uncertainty (S/U) analyses
- **Tungsten**
  - structural material present in process facilities and also of essential importance for shielding
  - long-standing computational bias associated with tungsten in benchmark calculations (poor performance of capture data)
  - Need for evaluated covariance data for S/U analyses

^{40}Ca Cross Section Evaluation Overview
(in ENDF/B-VII.1 library)

- Current status of ^{40}Ca evaluation in ENDF/B-VII.1 library (2011)
  - Evaluation work taken from JEFF-3.1 (May 2005, A.J. Koning)
  - Original data taken from JEFF-3.1 (Oct. 2004)
    - Resonance parameters (MF2/MT151) : JENDL-3.3 (2002) for E< 500 keV
    - Total cross section (MF3/MT1) : ENDF/B-VI.8 (2001) for E< 20 MeV
    - All other data : produced by TALYS code (May 2005)
- In ENDF/B-VII.1 library resonance parameters for Multi Level Breit Wigner formula taken from the recommended data (Mughabghab, 1981)
- No covariance data given in the ENDF/B-VII.1 library

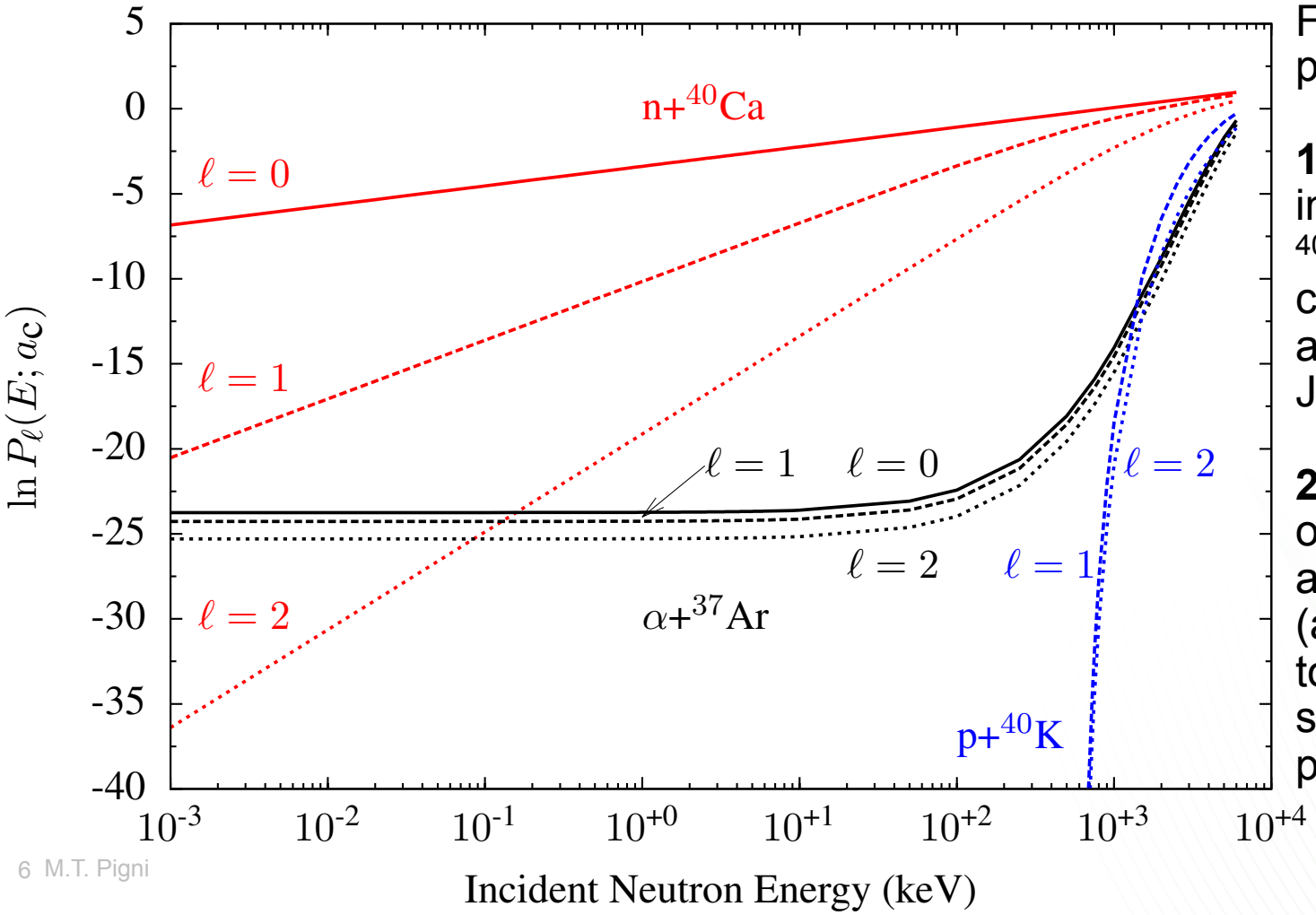
^{40}Ca Cross Section Evaluation Overview
(reaction channels)

Reaction product	Q-value (keV)	Threshold (keV)
^{41}Ca+γ	+8362.82	0.0
^{37}Ar+α_0	+1747.66	0.0
^{40}K+p_0	-528.55	541.89
^{40}Ca+n_1	-3352.62	3437.17
^{39}Ca+2n	-15635.0	16029.74

- Besides the elastic channel, three reactions (in red) are energetically possible in the neutron energy region up 1.5 MeV
  - α-particle emissions (Q-value>0) also at sub-thermal and thermal energies
- For charged particle reaction channels penetrability factors defined by the Coulomb functions F_l and G_l : $P_l=\rho/(F_l+G_l)$

n+^{40}Ca Channel Definitions
(particle pairs)

- The magnitude of the penetrability factors determines the strength of the partial-wave components of the quasi-stationary compound state.



For p+^{40}K particle-pair

1) *s*-wave are not included because ^{40}K has spin $I^{\pi}=4^-$ coupling to have total angular momentum $J^{\pi}=7/2^-$ and $9/2^-$

2) careful treatment of the partial widths at threshold energies (about 0.5 MeV) due to the considerable small values of the penetrability factors

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n+^{40}Ca Resonance Evaluation

- Transmission and capture cross section measurements performed at Geel for ^{nat}Ca in the energy range up to 1 MeV (Guber)
  - Measurements of Calcium using metallic samples
  - The samples are in Al canning due to reactivity with air
  - Transmission experiments w/ different sample thickness (flight path 50 m)
  - Neutron capture using detector system (flight path 60 m)

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- Early high-resolution total cross section measurements by
  - Cierjacks (1968, KIT): ^{nat}Ca(n,tot)
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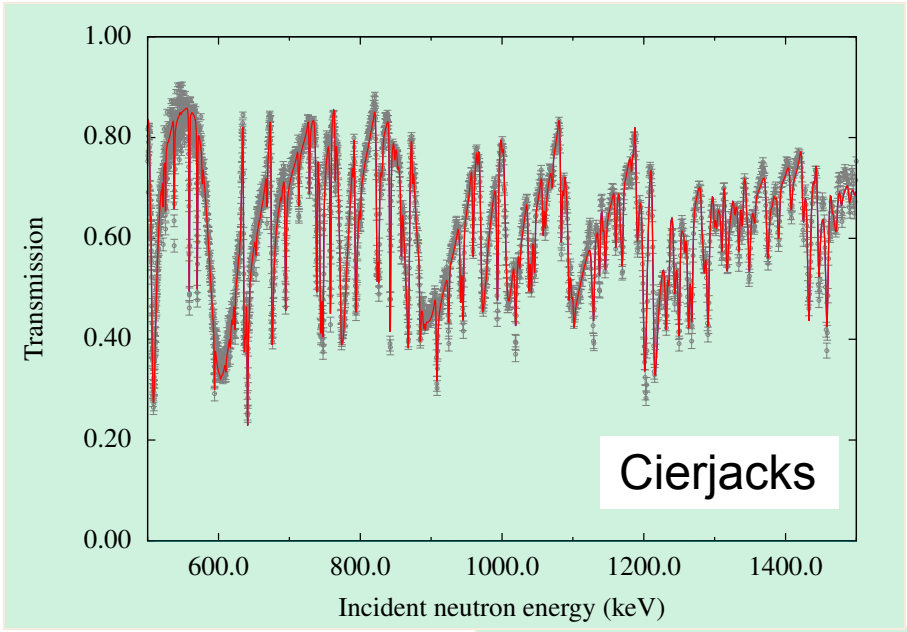
- Used formalism of Reich-Moore approximation
- Included (n,α) and (n,p) channels

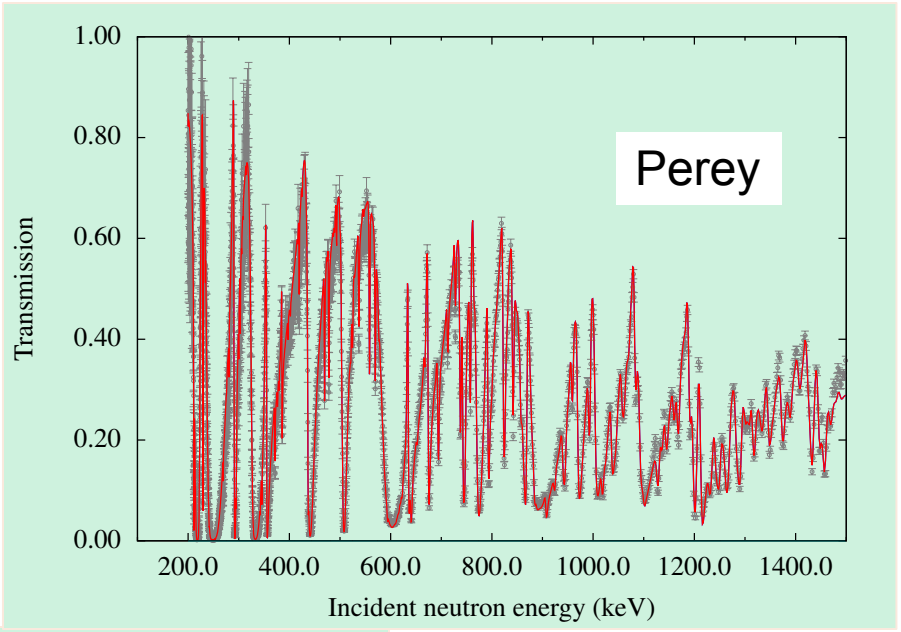
n+^{40}Ca Experimental Data Overview

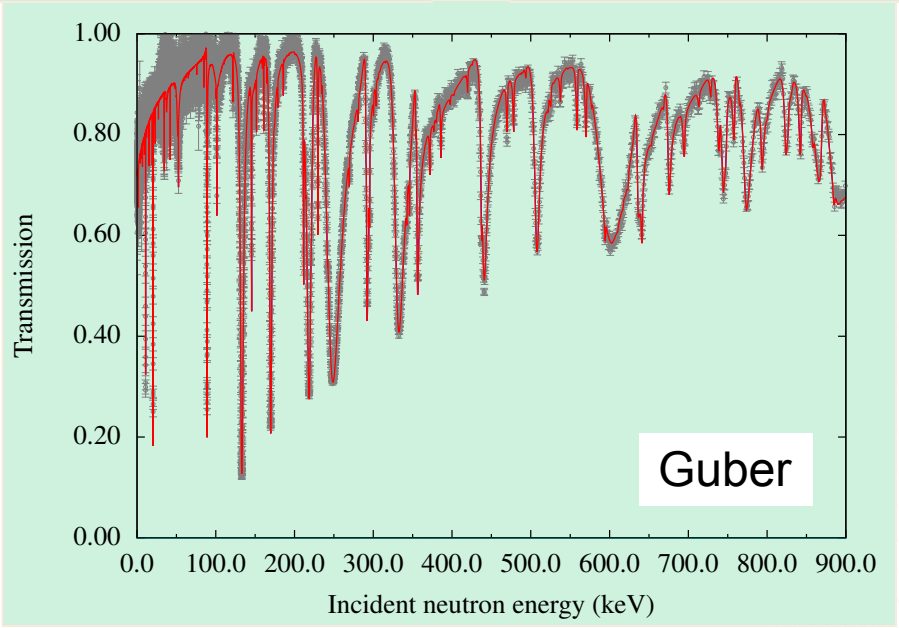
Sample	Author (Fac./Year)	Exp. range (keV) E_{fit}	Reaction Thick.(at/b)	No. data (No. data E_{fit})	X^{2**} (ave. unc.)
^{nat}Ca*	Cierjacks (KIT/1968)	500-31000 (1500)	Total 0.21326	5113 (2476)	5.39 (1.5%)
^{nat}Ca*	Perey (ORNL/1972)	200-29000 (1500)	Total 0.7028	3501 (2420)	2.07 (16.4%)
^{40}Ca*	Johnson (ORNL/1973)	40-6000 (1500)	Total 0.0656	7709 (6502)	6.12 (3.8%)
^{nat}Ca*	Singh (NSC/1974)	1.6-550 (550)	Total 0.029762	674 (674)	4.15 (10.0%)
^{nat}Ca	Guber (GEEL/2014)	0.02-1000 (900)	Trans 0.10971	28764 (28672)	1.08 (2.6%)
^{nat}Ca	Guber (GEEL/2014)	0.02-600 (350)	Capture 0.01674	20776 (19930)	1.42 (14.8%)
^{nat}Ca	Guber (GEEL/2015)	0.01-600 (350)	Capture 0.10971	17316 (16471)	1.86 (17.2%)

* Retrieved from EXFOR library
** up to 1500 keV

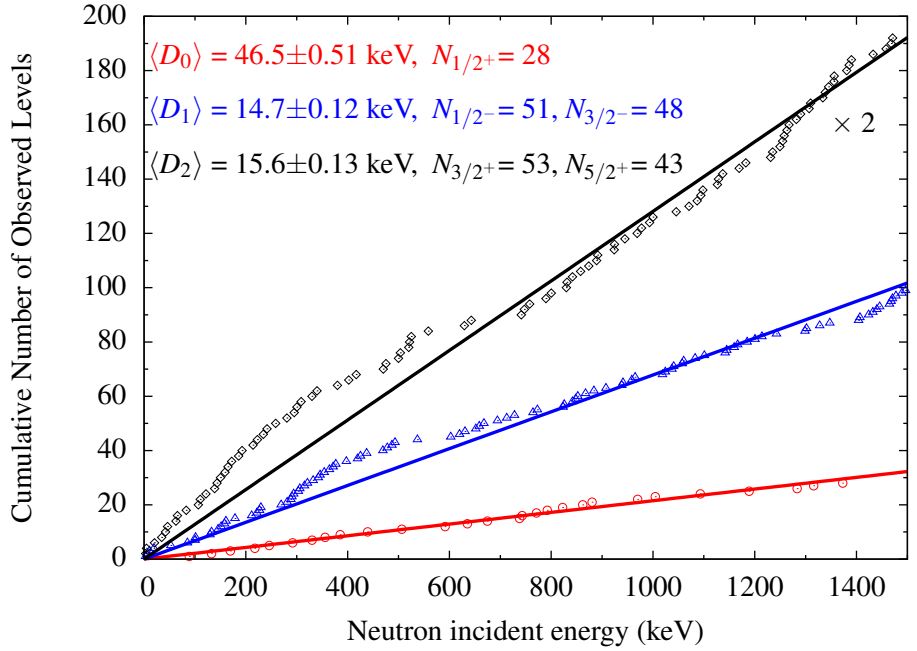
n+^{40}Ca Cross section evaluation work
(results)

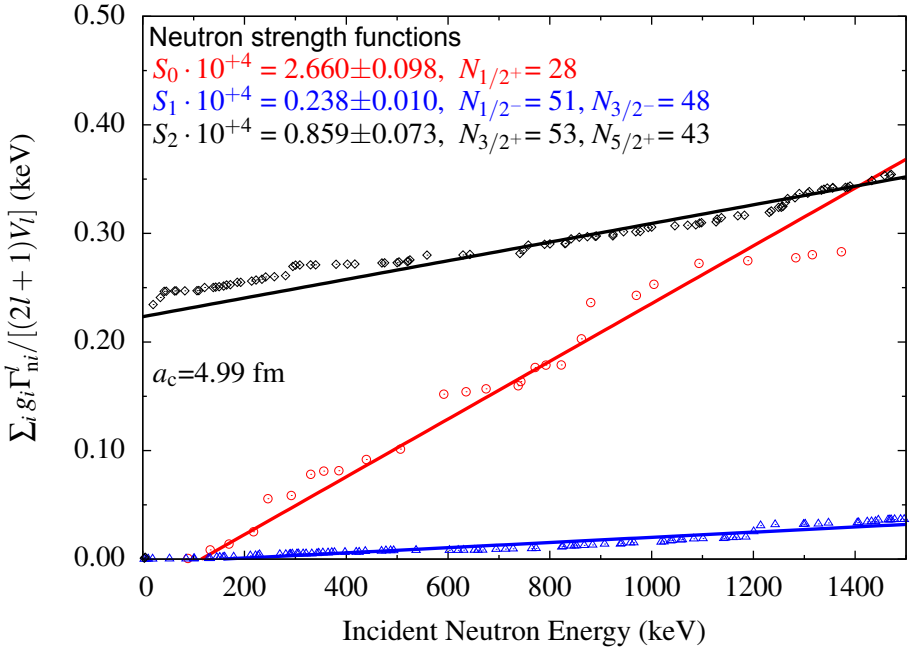


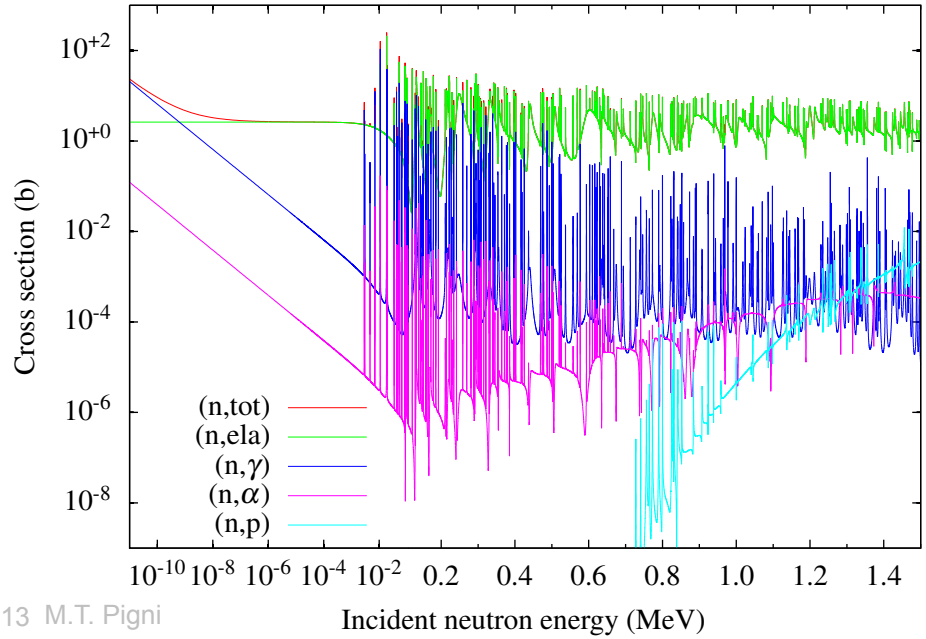




n+^{40}Ca evaluation statistics







- 7 experimental data sets (5 transmission and 2 capture) included in the cross section evaluation up to 1.5 MeV
- 5 reaction channels (2 for charged-particle emission)
- Total number of levels : 223
- Reich-Moore formalism used
- ENDF format : LRF=7, LCOMP=1

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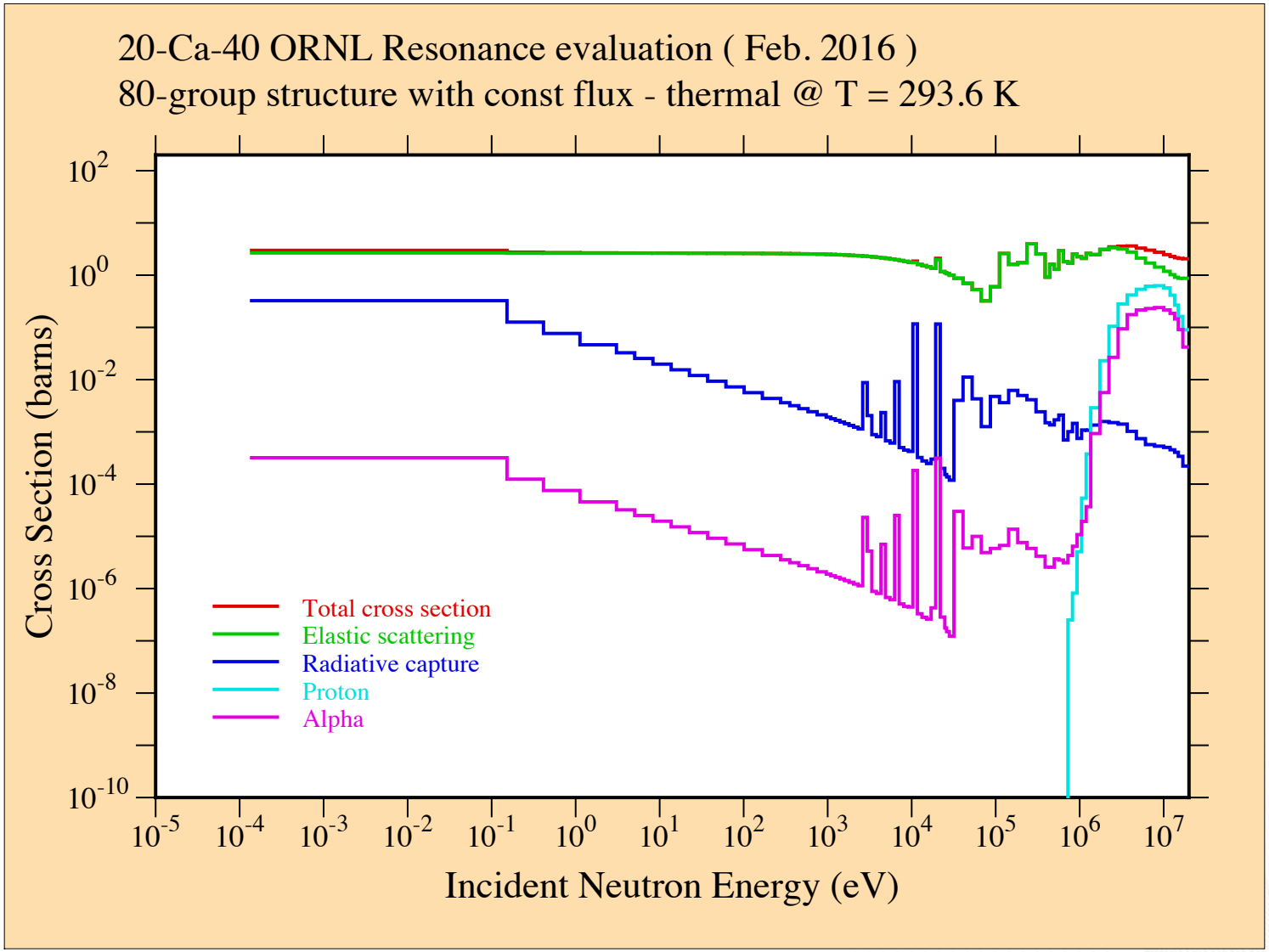
n+^{40}Ca cross section (up to 20 MeV) and covariances (up 1.5 MeV)



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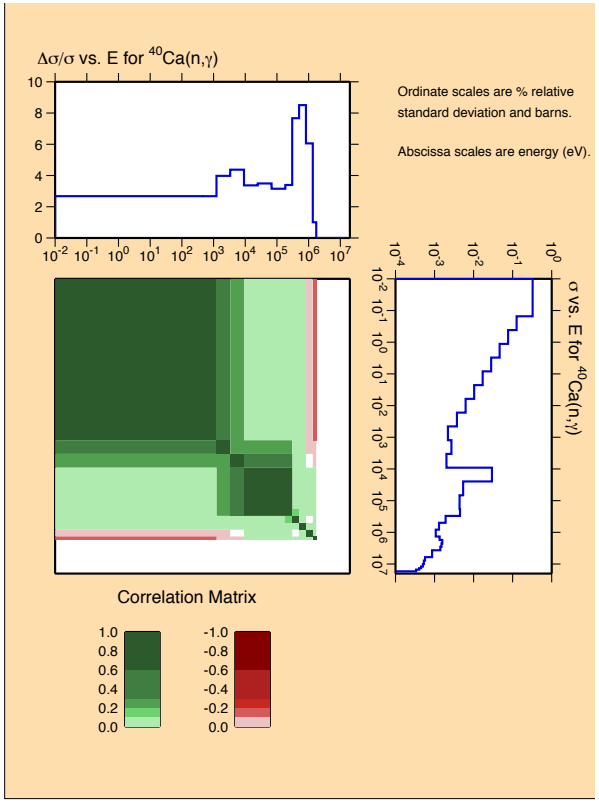
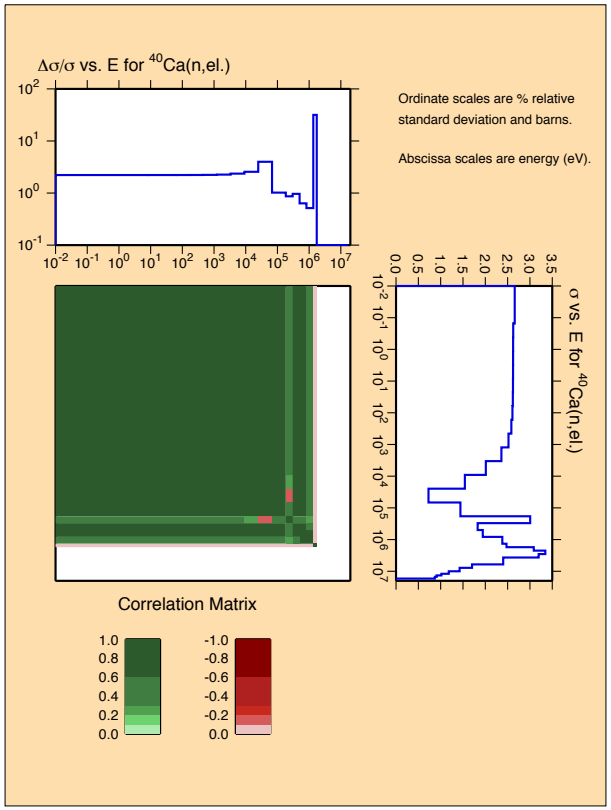
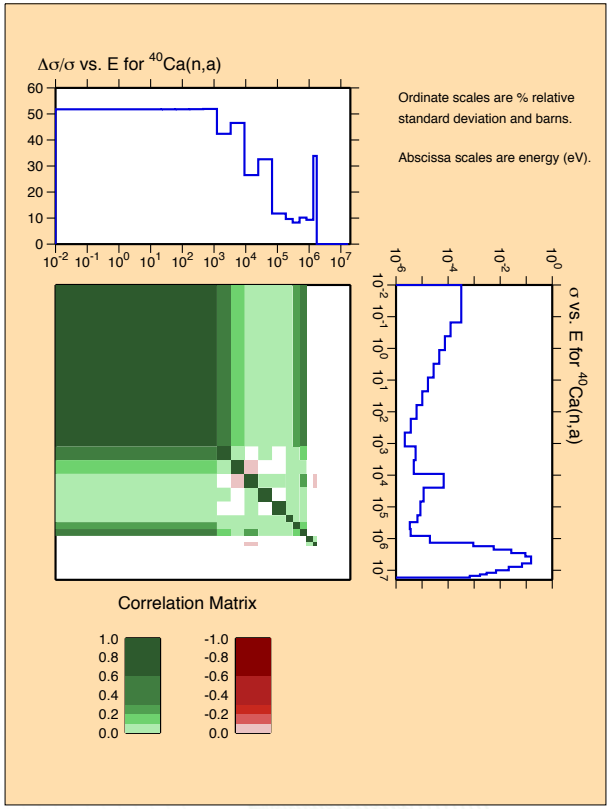


Capture-Capture



Elastic-Elastic



α-α

33-group representation (T=293.6 K)

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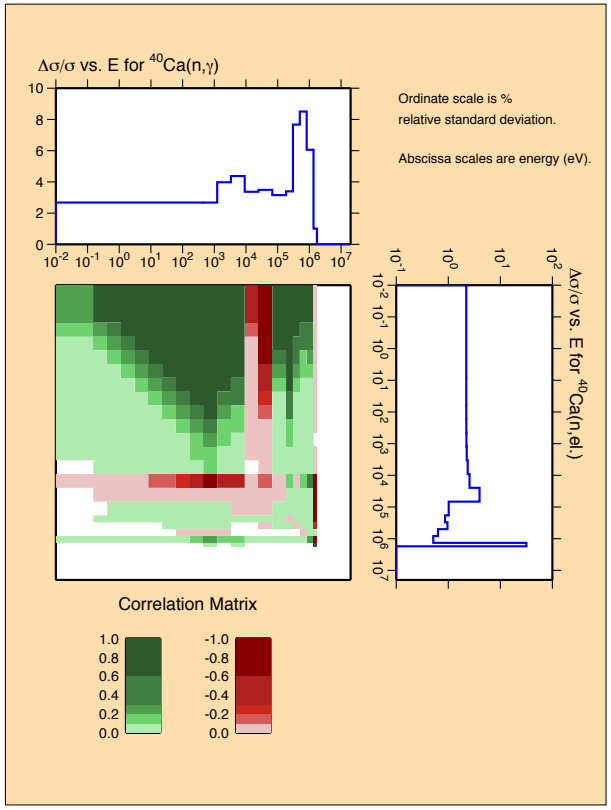
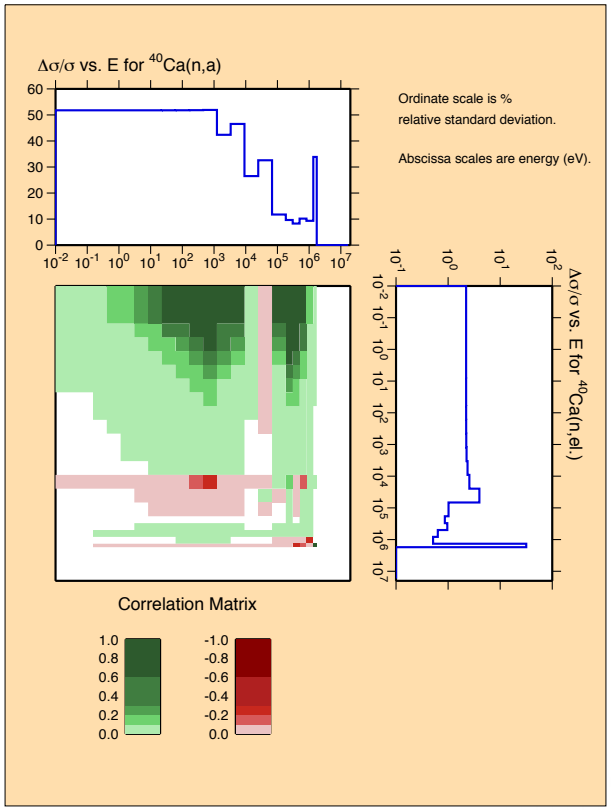
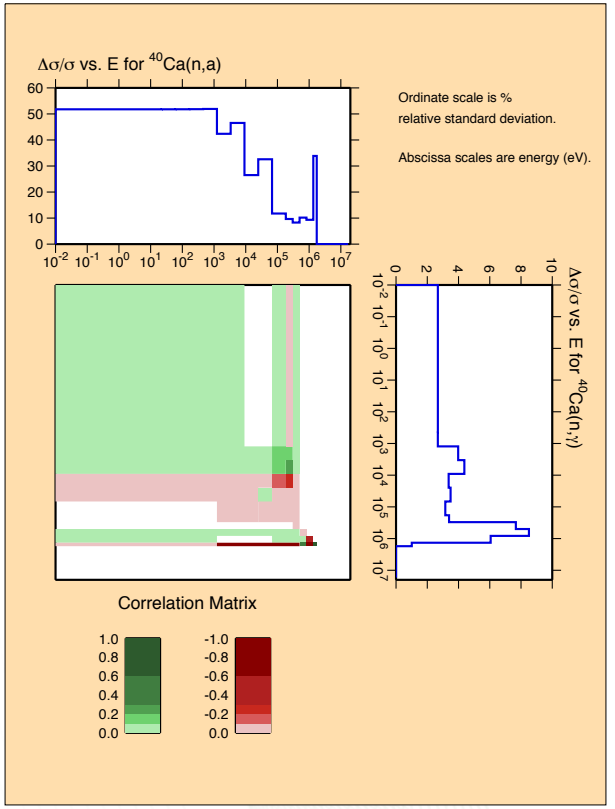
n+^{40}Ca cross section (up to 20 MeV) and covariances (up 1.5 MeV)



Capture-Elastic



α-Elastic



α-Capture

33-group representation (T=293.6 K)

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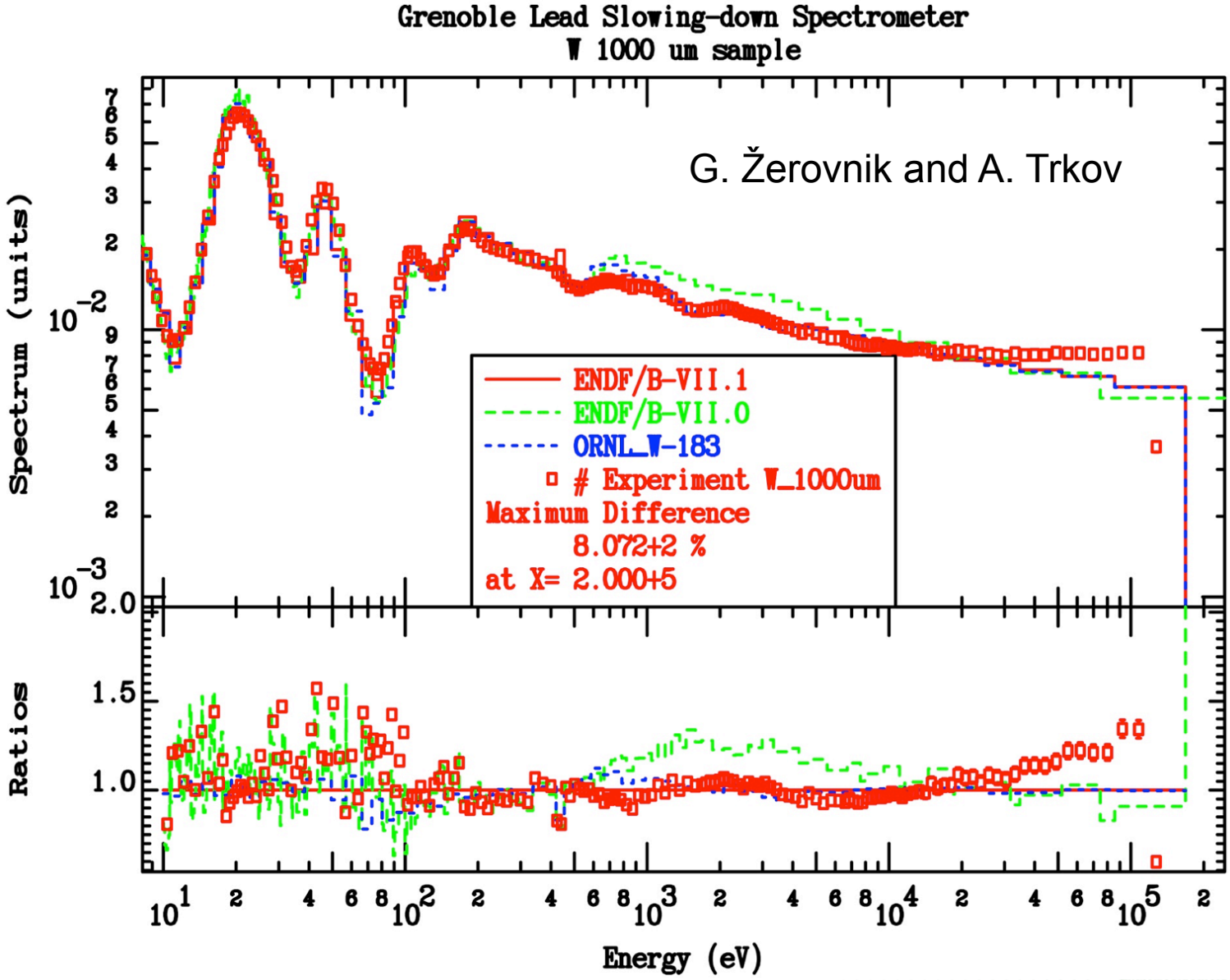
Validation of Tungsten Evaluations

- Four Tungsten evaluations, namely $^{182,183,184,186}W$, were completed in August 2014
- Three reference published papers
  - M.T. Pigni et al., PHYSOR 2012 - Knoxville, TN April 15-20 2012
  - M.T. Pigni et al., International Conference on Nuclear Data for Science and Technology (ND2013), New York, NY March 4-8 2013
  - M.T. Pigni et al., International Conference on Nuclear Criticality Safety (ICNC2015), Charlotte, NC September 13-17, 2015
- Preliminary validation on ^{183}W in 2013
- Validation on the set of four tungsten evaluations started in November 2015 (thanks to G. Žerovnik, IRMM)
  - Submitted paper to ND2016.

Preliminary validation on ^{183}W (2013)



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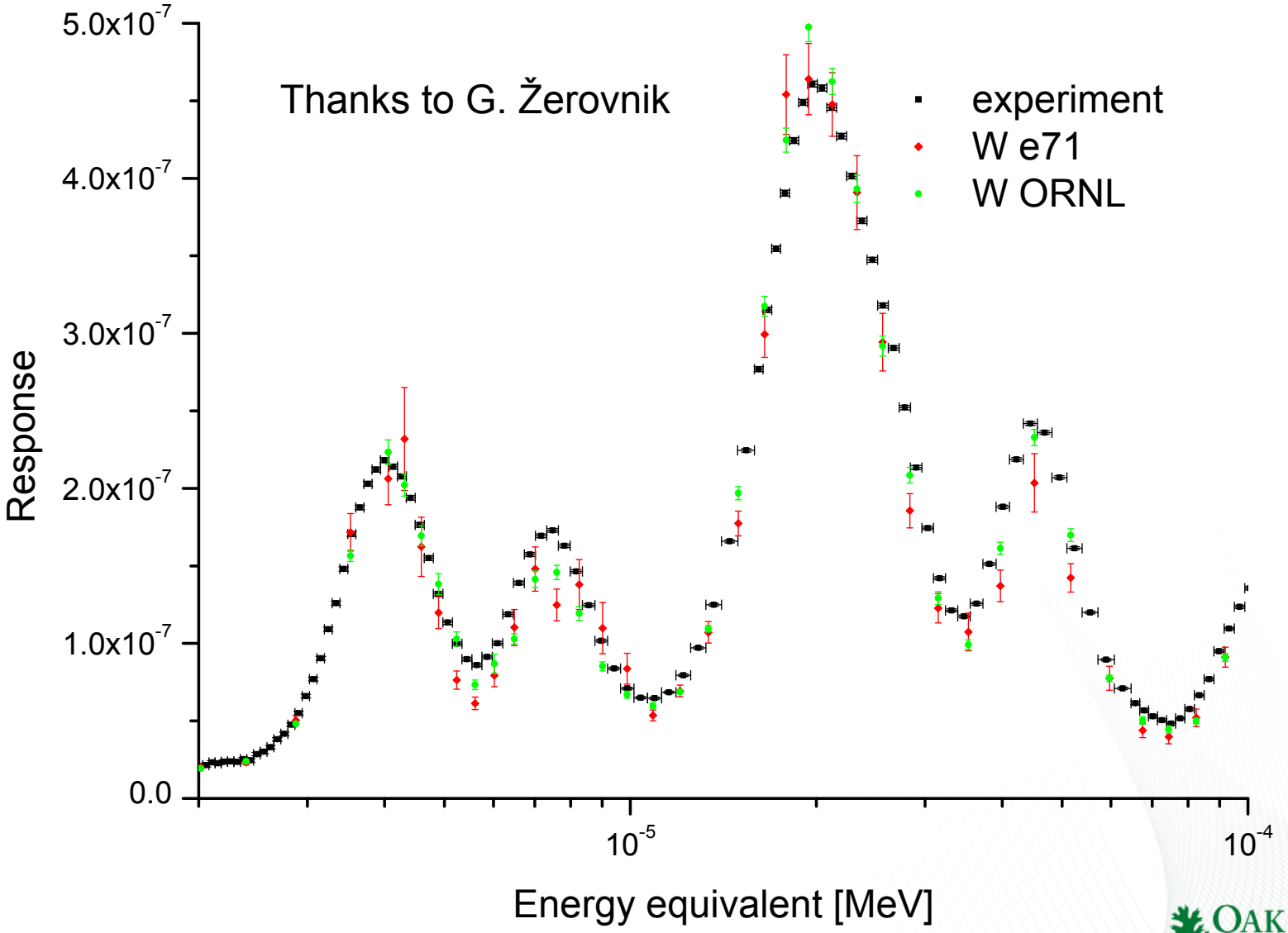
Validation of Tungsten evaluations (2015)
(Grenoble Lead Slowing down Spectrometer)



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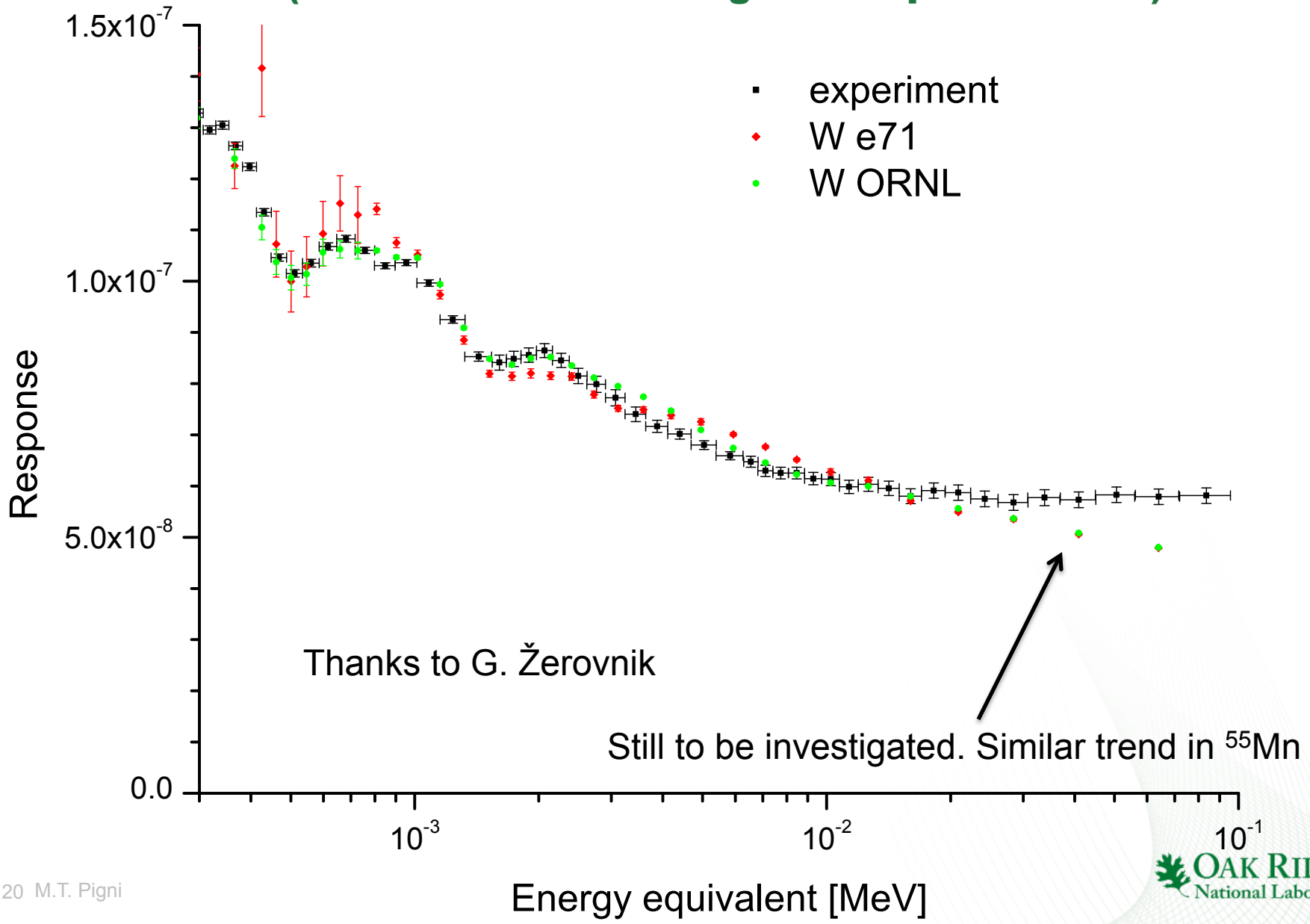

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Summary and Conclusions

- We applied the R-matrix SAMMY method using the Reich-Moore approximation to determine a consistent set of neutron resonance parameters and related covariance matrix for ^{40}Ca
- In the analyzed energy range up to 1.5 MeV, the evaluation *triples* the RRR energy range present in the latest US nuclear data library (ENDF/B-VII.1)
- 7 experimental data sets were used to ensure the calculated cross sections were in good agreement with multiple transmission (5) and capture data (2) sets
- Results agree with the systematics of the observed s-, p-, and d-wave resonances, such as level spacing systematics and strength functions
- Charged-particle reaction channels, such as (n,a) and (n,p), were also included in the evaluation
- Calcium evaluated file (LRF=7) also include covariance matrix for the resonance parameters (LCOMP=1)
- Internal repository (GIT) for all SAMMY inputs and experimental data sets was created within ORNL Gitlab server
- For tungsten evaluations, the validation analysis on the Grenoble LSD benchmark showed an improved agreement with the experimental response when the new evaluations were included in the ENDF/B-VII.1 library

ACKNOWLEDGMENTS

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Thank you!